

ICCDU VI
Sunday September 9-Friday September 14, 2001
Breckenridge, Colorado, USA

Conference Program

Sunday, September 9

4:00 PM-7:00 PM Registration and Reception

Monday, September 10

7:00 AM – 7:45 AM Continental Breakfast

7:00 AM – 5:30 PM Registration

Welcome/ Opening Session

Donald Darensbourg/Dan DuBois, Chairs

7:45 AM – 8:00 AM Stanley R. Bull Director of Science and Technology, National Renewable Energy Laboratory

8:00 AM – 8:45 AM PL-1. Michele Aresta and Angela Dibenedetto, "Carbon Dioxide Utilization in Developing Innovative Synthetic Methodologies"

8:45 AM – 9:30 AM PL-2. Edward Dlugokencky, "The Global Carbon Cycle and its Role in Climate Change"

9:30 AM – 10:15 AM K-3. Eric Beckman, "Copolymerization of CO₂ and Cyclic Ethers"

10:15 AM – 10:30 AM Coffee Break

Chemicals From CO₂

Kenneth Nicholas, Chair

10:30AM – 10:55 AM O-4. Shohei Inoue, "Reaction of Carbon Dioxide and Epoxide Controlled by Light with a Metalloporphyrin-Base System"

10:55 AM – 11:20 AM O-5. Peter Groll, Achim Jansen, Doreen Krolle and Stephan Pitter, "Atmospheric Pressure Hydrosilylation of Carbon Dioxide"

11:20 AM – 11:45 AM	O-6. Michele Aresta and <u>Angela Dibenedetto</u>, "Enantioselective Nb-Catalyzed Synthesis of Organic Cyclic Carbonates Based on Carbon Dioxide Utilisation"
11:45 AM – 12:10 PM	O-7. <u>Larisa G.Tomilova</u>, Evgeniya G. Kogan, Alexey V. Ivanov and Nikolai S. Zefirov, "Applications of Phthalocyanine Complexes for Carbon Dioxide Fixation"
12:10 PM – 1:15 PM	Lunch on your own
<u>Chemicals From CO₂</u>	Eric Beckman, Chair
1:15 PM – 1:40 PM	O-8. <u>Yoshiyuki Sasaki</u> and Ken-ichi Tominaga, "Synthesis of 2-Oxazolidinones from CO₂ and 1,2-Aminoalcohols Catalyzed by <i>n</i>-Bu₂SnO"
1:40 PM – 2:05 PM	O-9. <u>Mahmut Abla</u>, Jun-Chul Choi, and Toshiyasu Sakakura, "Halogen-Free Process for the Conversion of Carbon Dioxide to Urethanes by Homogeneous Catalysis"
2:05 PM – 2:30 PM	O-10. <u>Ken-ichi Tominaga</u> and Yoshiyuki Sasaki, "Hydroformylation Using Carbon Dioxide as a Reactant"
2:30 PM – 2:55 PM	O-11. <u>C. Wolff</u>, T. Oberreuther, A. Behr, "Utilization of Carbon Dioxide Using a Non-equilibrium, Microwave-induced Plasma at Atmospheric Pressure"
2:55 PM – 3:20 PM	O-12. S. L. Yao, M. Okumoto, A. Nakayama, and <u>E. Suzuki</u>, "Plasma Reduction of Carbon Dioxide with Methane"
3:20 PM – 3:35 PM	Refreshment Break
<u>Supercritical/Dense Phases</u>	Robert Klingler, Chair
3:35 PM – 4:20 PM	K-13. <u>William Tumas</u>, "Dense Phase Carbon Dioxide as a Reaction Medium for Homogeneous and Biphasic Catalysis"
4:20 PM – 4:45 PM	O-14. <u>D. Ballivet-Tkatchenko</u>, T. Jerphagnon, and H. Chermette, "Synthesis of Dialkyl Carbonates from Alcohols and CO₂ under Supercritical Conditions"
4:45 PM – 5:10 PM	O-15. <u>Philip G. Jessop</u>, John C. Linehan, A. Denise Main, Justine M. Pitts, Chih-Cheng Tai, Pradip Munshi, "Recent

Developments in the Hydrogenation of CO₂ Catalyzed by Ruthenium Phosphine Complexes"

Tuesday, September 11

7:00 AM – 8:00 AM

Continental Breakfast

7:00 AM – 5:00 PM

Registration Desk Open

**Supercritical/
Dense Phases**

8:00 AM – 8:45 AM

Philip G. Jessop, Chair

PL-16. E. Dinjus, "Carbon Dioxide as C₁ Building Block"

8:45 AM – 9:30 AM

PL-17. Joseph M. DeSimone, "The CO₂ Technology Platform: Surfactants for Increased CO₂ Utility"

9:30 AM – 9:55 AM

O-18. Daniel M. Blake, Steven Phillips, Calvin Feik, John Scahill, and Debra L. Bryant, "Photocatalytic Oxidation of Organic Compounds on Titania in Supercritical Carbon Dioxide"

9:55 AM – 10:20 AM

O-19. Klaus Woelk, "Colloid-Catalyzed Single-Phase Hydrogenation in Supercritical CO₂"

10:20 AM – 10:30 AM

Coffee Break

**Supercritical/
Dense Phases**

10:30AM – 10:55 AM

Daniel M. Blake, Chair

O-20. Robert J. Klingler, Jerome W. Rathke, Michael J. Chen, and Rex E. Gerald II, "High-Pressure NMR Studies in Supercritical Media"

10:55 AM – 11:20 AM

O-21. Dongil Lee, John C. Hutchison, Jason S. Keiper, Joseph M. DeSimone and Royce W. Murray, "Transport of Micelles and Monomeric Solutes in Supercritical CO₂"

11:20 AM – 11:45 AM

O-22. Fabrice Stassin and Robert Jérôme, "Ring-Opening Polymerization of Cyclic (Di)esters in Supercritical Carbon Dioxide"

11:45 AM – 12:10 PM

O-23. A. P. Fonseca, M. F. Mendes, F. L. P. Pessoa, and A. M. C. Uller, "The Uses of Carbon Dioxide in Supercritical Technology Researches in Brazil"

12:10 PM – 1:15 PM

Lunch on your own

12:15 PM – 10:00 PM	Set up Posters
<u>General CO₂</u>	Calvin Curtis, Chair
1:15 PM – 1:40 PM	O-24. Jason Yarbrough and Donald J. Darensbourg, "The Use of Schiff-Base Complexes for the Catalysis of Carbon Dioxide and Epoxide Copolymerization"
1:40 PM – 2:05 PM	O-25. G. Laurenczy, F. Joó, and L. Nádasdi "Catalytic CO₂/HCO₃⁻ Reduction in Aqueous Solutions"
2:05 PM – 2:30 PM	O-26. Kazuhiko Ichikawa and Kou Nakata, "CO₂-Encapsulated Clathrate Hydrate Formed by Sulfonate-Assisting Hydrogen Bonds and Template Contribution from Helper Species of Zinc(II)"
2:30 PM – 2:55 PM	O-27. Manfred Doering, Michael Ciesielski, and Olaf Walter, "Zinc Schiff Base Complexes for CO₂ Fixation: Enzymatic Models of CO₂ Reactions"
2:55 PM – 3:20 PM	O-28. William W. Ellis, Calvin J. Curtis, Douglas E. Berning, Dorothy H. Gibson and Daniel L. DuBois, "Reduction of CO₂ and Coordinated CO Using Transition-Metal Hydrides"
3:20 PM – 3:35 PM	Refreshment Break
<u>Biological/ Biochemical</u>	Stephen Ragsdale, Chair
3:35 PM – 4:20 PM	PL-29. Masaharu Ishii, Songkran Chuakrut, Yun Rarae, Ayako Nishiyama, Masahiro Yamamoto, Hiroyuki Arai, and Yasuo Igarashi, "Genes and Proteins Involved in Carboxylation Reactions from Autotrophs with Non-Calvin Type CO₂ Fixation Pathway"
4:20 PM – 5:05 PM	I-30. James G. Ferry, "Structural and Mechanistic Diversity of Prokaryotic Carbonic Anhydrases"

Wednesday, September 12

7:00 AM – 8:00 AM	Continental Breakfast
7:00 AM – 5:00 PM	Registration Desk Open
<u>Biological/ Biochemical</u>	James G. Ferry, Chair
8:00 AM – 8:45 AM	PL-31. <u>Lars G. Ljungdahl</u>, "Microbial CO₂ Fixation: An Overview"
8:45 AM – 9:30 AM	PL-32. <u>K. Izui</u>, H. Matsumura and Y. Kai, "Phosphoenolpyruvate Carboxylase: Three Dimensional Structure, Reaction Mechanism and Regulation"
9:30 AM – 10:15 AM	I-33. <u>Michael J. Russell</u> and Allan J. Hall, "The Onset of Life and the Dawn of Oxygenic Photosynthesis: Respective Roles of [Fe₄S₄]²⁺ Cubane and Transient [Mn₄O₄]⁶⁺ in CO₂ Reduction
10:15 AM – 10:30 AM	Coffee Break
<u>Biological/ Biochemical</u>	Lars Ljungdahl, Chair
10:30AM – 11:10 AM	I-34. <u>Stephen W. Ragsdale</u>, "From One Greenhouse Gas to Another: the Biological Conversion of CO₂ To Methane"
11:10 AM – 11:50 AM	I-35. <u>Robert J. Spreitzer</u>, "Rubisco: How to Make a Better CO₂-Fixing Enzyme"
11:50 AM – 12:30 PM	I-36. <u>Stephen P. Long</u>, Abdul K. Al-Shoaibi, Clive V. Beale, John Clifton-Brown, Emily A. Heaton, Michael B. Jones and S. Naidu, "Enhancing CO₂ Utilization and Potential Sequestration in Temperate Climates with C4 Photosynthesis: Theoretical Analysis and Practical Experience with <i>Miscanthus</i>"
12:30 PM – 1:30 PM	Scientific Committee Meeting/Lunch
	Afternoon Free
7:00 PM – 9:00 PM	PO-1 – PO-28 Poster Session and Reception

Posters

Dimensions: 4' x 8' or 1.22m x 2.43m

Setup Tuesday 12:15pm – 10:00pm
Take Down No Later Than 1:00pm Thursday

- PO-1.** M. Jason Adams and Donald J. Dahrensbourg, “The Use of Double Metal Cyanides for the Coupling of Epoxides and CO₂”
- PO-2.** R. Akhmedov, E. Akhmedov, B. Barochin, “Economic Advantages of Technology of Burning Fuel with Way Production and Effective Utilization of CO₂”
- PO-3.** S. Aoyagi, Y. Utsumi, M. Matsudaira, T. Yamamoto, T. N. Rao, D. A. Tryk, A. Fujishima, “Electrochemical Reduction of CO₂ in High Pressure CO₂-Methanol Systems”
- PO-4.** Michele Aresta, Immacolata Tommasi, Caterina Dileo e, Angela Dibenedetto, “Reaction of Ketals with Carbon Dioxide in Organic Solvents and in Sc-CO₂”
- PO-5.** A. V. Baburin, I. R. Begishev, A. K. Belikov, P. V. Komrakov, “The Parameters of Methane Kinetic Burning in the Oxidation Medium (O₂ + CO₂)”
- PO-6.** D. Ballivet-Tkatchenko and H. Chermette, “DFT Modeling of CO₂ Uptake and Dimethyl Carbonate Formation with Methoxymethylstannanes”
- PO-7.** S. Camy, D. Ballivet-Tkatchenko, and J.-S. Condoret, “Process of Dimethyl Carbonate Synthesis Using Supercritical Carbon Dioxide: Study and Modeling of the Reacting Mixture Fractionation”
- PO-8.** Elena Caterina Celia, Enrico Cernia, Cleofe Palocci, Simonetta Soro, and Tiziana Turchet, “Supercritical Fluids as Reaction Media Useful to Modulate *Pseudomonas Cepacia* Lipase Activity in Transesterification Reactions”
- PO-9.** Huey-Ing Chen, Hong-Yi Chang, Po-Hung Chen, Edward T. S. Huang, “High-Pressure Phase Equilibria of Carbon Dioxide- Water- *n*-Butanol System”
- PO-10.** Jun-Chul Choi, Hiroyuki Yasuda, Toshiyasu Sakakura, “Catalytic C-H Bond Activation by the RhCl(PMe₃)₃-*hν* System in Dense Carbon Dioxide”
- PO-11.** Micro Costa and Andrea Arisi, “1,3-Oxazolidin-2-one Ring Formation from Carbon Dioxide and N-alkyl-g-aminocrotonate under Homogeneous and Supercritical Conditions”
- PO-12.** C. Curtis, A. Miedaner, J. Turner, W. Ellis, B. Cox, and D. L. DuBois, “Rapid-Throughput Studies of Bimetallic CO₂ Reduction Catalysts”

- PO-13.** M. F. Davis, S. R. Thomas, G. A. Tuskan, S.D. Wullschleger, T.J. Tschaplinski, L.E. Gunter, M. M. Sewell, D. B. Neale and N.C. Wheeler, “Carbon Allocation and Partitioning in Woody Plants: A Means to Enhance Bioenergy Conversion and Carbon Sequestration.”
- PO-14.** R. Fiorentini, G. Andrich, A. Zinnai, S. Balzini, and F. Venturi, “Supercritical Fluid Extraction of Polyphenols from By-Products of Potato Industry”
- PO-15.** Russell J. Franks and Kenneth M. Nicholas, “Metal-Promoted Carboxylative Coupling of Organometals and Organic Electrophiles”
- PO-16.** M. Halmann, A. Frei, and A. Steinfeld, “Avoidance of Carbon Dioxide Release by Combining Metal Oxide Reduction with Partial Methane Oxidation in a Thermo-neutral Process”
- PO-17.** Wolfgang Kaim, Michael Weber, Thomas Scheiring, Matthias Wanner, and Jan Fiedler, “Primary Activation Processes of Heterodinuclear Complex Ions [$(h^5\text{-C}_5\text{Me}_5)\text{ClM}(\mu\text{-L})\text{Re}(\text{CO})_3\text{Cl}]^+$, M = Rh or Ir, for the Reductive CO_2/H^+ Conversion”
- PO-18.** Hajime Kawanami and Yutaka Ikushima, “Direct Urethane Synthesis by the Reaction of Aminoalcohol with Carbon Dioxide under Supercritical Conditions”
- PO-19.** Samuel J. Lewis and Donald J. Darensbourg, “Lewis Base Adducts of Zinc Complexes for the Coupling of CO_2 and Epoxides”
- PO-20.** Kou Nakata, Naomi Shiina, Mitunori Izumi, M. M. Ibrahim, Kazuhiko Ichikawa, and Motoo Shiro, “Kinetic Study of Catalytic CO_2 Hydration by Water-Soluble Model Compound of Carbonic Anhydrase and Anion Inhibition Effect on CO_2 Hydration”
- PO-21.** Heiko G. Niessen, Peter Trautner, and Klaus Woelk, “*In Situ* NMR Studies and Diffusion Imaging in Supercritical CO_2 ”
- PO-22.** Kiyomi Okabe, Hidekazu Yamada, Takaaki Hanaoka, Takehiko Matsuzaki, Hironori Arakawa, and Yoshimoto Abe, “ CO_2 Hydrogenation to Methanol and Ethanol over Highly Dispersed Co/SiO₂ Catalysts Derived from Acetate”
- PO-23.** Joseph C. Poshusta, Daniel L. DuBois, Carl A. Koval, and Richard D. Noble, “Electrochemical Separation of CO_2 Mixtures”
- PO-24.** M. Saito, N. Mimura, I. Takahara, J. Wu, and H. Kimura, “Catalytic Dehydrogenation of Hydrocarbons in the Presence of Carbon Dioxide”
- PO-25.** U. Storzer, O. Walter, E. Dinjus, “Stereochemical Control of Coupling Butadiene and CO_2 at Palladium Centres”

- PO-26. Djoko Suwasono, "Potential Clean Development Mechanism Program in Pertamina - Indonesia"**
- PO-27. G. Peter van Walsum, "Comparison of Carbon Dioxide and Sulfer Dioxide for Acid-Catalyzed Steam Explosion of Biomass: A Thermodynamic Investigation"**
- PO-28. G. D. Zakumbaeva, L. B. Shapovalova, A. N. Gabdrakipov, A. A. Zhurtbaeva, I. S. Chanisheva, L. V. Komashko, "The Effect of the Support Nature on the Properties of Ru-Co-catalysts in CO₂ + C₃H₆ Reaction"**

Thursday, September 13

7:00 AM – 1:00 PM	Remove Posters (Anything not removed by 1:00 PM may be thrown away.)
7:00 AM – 8:00 AM	Continental Breakfast
7:00 AM – 5:00 PM	Registration Desk Open
<u>Homogeneous and Electrochemical Reductions</u>	Etsuko Fujita, Chair
8:00 AM – 8:45 AM	PL-37. Masahiro Isaka and <u>Hironori Arakawa</u>, "Effective Synthesis of Ethanol by Catalytic Hydrogenation of CO₂ Using Ru₃(CO)₁₂-CO₂(CO)₈-LiBr-Bu₃PO System"
8:45 AM – 9:30 AM	PL-38. <u>Koji Tanaka</u>, "Metal-Carbon Bond Character of Reaction Intermediates in Multi-electron Reduction of CO₂ Catalyzed by Ruthenium Complexes"
9:30 AM – 9:55 AM	O-39. <u>Dorothy H. Gibson</u> and Haiyang He, "Synthesis and Properties of <i>fac</i>-Re(dmbpy)(CO)₃CHO (dmbpy = 4,4'-dimethyl-2,2'-bipyridine), a Possible Intermediate in Reductions of CO₂ Catalyzed by <i>fac</i>-Re(dmbpy)(CO)₃Cl"
9:55 AM – 10:20 AM	O-40. <u>Woonsup Shin</u>, Yousung Kim, Hojun Lee, Misuk Cho, Miran Lim, Sang Phil Lee, Ji Sun Kim, Sang Hee Lee, and Jun Won Shin, "Electrochemical Activation of Carbon Dioxide to Carbon Monoxide or Acetate by Enzymes in <i>Clostridium Thermoaceticum</i>"
10:20 AM – 10:30 AM	Coffee Break

Photoreduction

10:30AM – 10:55 AM

Dorothy Gibson, Chair

O-41. Etsuko Fujita, Kazuteru Shinozaki, Shoichi Kita, and Bruce S. Brunschwig, "Transient FTIR Study of Rhenium Complexes in Photochemical CO₂ Reduction"

10:55 AM – 11:20 AM

O-42. Hisao Hori, Yoko Suzuki, Kazuhide Koike, Koji Takeuchi, and Yoshiyuki Sasaki, "Application of High Pressure to Photocatalytic Carbon Dioxide Reduction Using Rhenium Complexes"

11:20 AM – 11:45 AM

O-43. Kiyohisa Ohta, Yuji Nisio, Satoshi Kaneco, and Toru Suzuki, "Photocatalytic Reduction of Carbon Dioxide by Goethite under Sunlight Irradiation"

11:45 AM – 12:10 PM

O-44. Heinz Frei, "Mechanistic Study of CO₂ Photoreduction in Ti Silicalite Molecular Sieve"

Posters down by 1:00PM

12:10 PM – 1:15 PM

Lunch on your own

Heterogeneous Reactions of CO₂

1:15 PM – 2:00 PM

Hironori Arakawa, Chair

K-45. Julian R. H. Ross, Erzeng Xue and Damien Treacy, "The CO₂ Reforming of Methane and Related Reactions"

2:00 PM – 2:25 PM

O-46. Thomas Riedel, Dominik Unruh, and Georg Schaub, "CO₂ Hydrogenation to Liquid Hydrocarbon Fuels"

2:25 PM – 2:50 PM

O-47. Shinichirou Morimoto, Wei Liu, Tsutomu Hayashi, Pyong Sik Pak, "Evaluation of Wind Energy Utilizing Methanol System"

2:50 PM – 3:15 PM

O-48. Son-Ki Ihm, Young-Kwon Park, Jong-Ki Jeon and Se-Won Baek, "CO₂ Hydrogenation over Cu-Containing Hybrid Catalysts for the Synthesis of Oxygenates"

3:15 PM – 3:30 PM

Refreshment Break

Heterogeneous Reactions of CO₂

3:30 PM – 3:55 PM

Thomas Riedel, Chair

O-49. F. Solymosi, L. Bugyi, A. Oszkó, and P. Tolmacsov, "Adsorption and Reaction of CO₂ on Mo₂C Catalyst"



3:55 PM – 4:20 PM

O-50. Sang-Eon Park, Jong-San Chang, Vladislav P. Vislovskiy, Min Seok Park, Kyoung Yul Lee, and Jin S. Yoo, "Dehydrogenation of Ethylbenzene with Carbon Dioxide: Effect of CO₂ as Soft Oxidant"

4:20 PM – 4:45 PM

O-51. Ki-Won Jun, Hyun-Seog Roh, Seung-Chan Baek, and Sang-Eon Park, "A Highly Effective Catalyst for CO₂ Reforming of Methane: Ni/Ce-ZrO₂?-Al₂O₃"

4:45 PM – 5:10 PM

O-52. Yihui Ding, Wei Huang, Ping Jin, and Kechang Xie, "Direct Synthesis of Acetic Acid from CO₂ and CH₄ over Supported Pd and Rh Catalysts"

6:30 PM – 9:00 PM

Banquet

Friday, September 14

7:00 AM – 8:00 AM

Continental Breakfast

7:00 AM – 11:30 AM

Registration Desk Open

Heterogeneous Reactions of CO₂

8:00 AM – 8:45 AM

PL-53. Kyu-Wan Lee, Ki-Won Jun, Sang-Sung Nam, Jin-Soo Hwang, Myoung-Jae Choi, "Catalytic Hydrogenation of CO₂ and CO₂ Rich Biosyngas to Clean Fuels"

8:45 AM – 9:30 AM

K-54. Klaus S. Lackner, "Managing the Global Carbon Cycle"

9:30 AM – 9:55 AM

O-55. Sh. S. Itkulova, G. D. Zakumbaeva, K. Z. Zhunussova and K. H. Nurgozhaev, "CO₂ Reforming of CH₄/Natural Gas over Supported Catalysts on the Base of the VIII Group Metals"

9:55 AM – 10:20 AM

O-56. Tahereh Kaghazchi, "Synthesis of Catalysts for Conversion of CO and CO₂ to Methanol"

10:20 AM – 10:35 AM

Coffee Break

10:35 AM – 11:15 AM

Conclusion